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The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.

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13. ABSTRACT (Maximum 200 words)

The objective of this research program is to study theoretically the underlying principles of quantum transport in solids. The specific areas of research are those of Bloch electron dynamics, quantum transport in oscillating electric fields or in periodic potentials, and the capacitive nature of atomic-size structures. A number of these problems are treated analyticaly to the extent possible through the use of dynamical localized Wannier functions.

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SUMMARY OF RESEARCH PROGRESS

During the contract period, we made much progress in the study of Bloch electron dynamics and quantum transport in solids. A brief description of each result is given below. More details can be found in our publications whose list is provided at the end of this section. Specifically, we have:

1) Derived a novel multi-band theory of Bloch electron dynamics in homogeneous electric fields of arbitrary strength. Generalized Zener tunneling time is obtained as a function of applied electric field and three-dimensional band parameters. The electric field-enhanced broadening of the excited state probability amplitudes and lattice space delocalization are investigated.

2) Analyzed the single-band and the multi-band proceses for a Bloch electron in the presence of a superimposed uniform and oscillating electric field. Resonant displacements of the Bloch electron and DC currents are observed including all possible transitions such as Zener tunneling, photon assisted tunneling, multiphoton emission/absorption, and transitions between Wannier Stark ladders.

3) Evaluated the transmission coefficient of a Bloch electron through impurity barriers in the one-dimensional nearest-neighbor tight-binding approximation. The electric field dependent Green's function was derived, and the Stark energy spectra under the influence of the impurities were calculated.

4) Developed a novel method of solving the multi-band quantum transport equation for a Bloch electron in spatially homogeneous electric field of arbitrary time dependence. The Wigner-Weisskopf approximation and the novel approximation lead to the analytical solutions which preserve the total probability.

5) Investigated the transmission of a Bloch electron through quantum barriers in spatially homogeneous, time-dependent electric field. The instantaneous basis were used in deriving the time and the electric field dependent transmission coefficients. The evolution of the wave packets through the tunneling structures in electric field were also examined.

REFEREED PUBLICATIONS

During the contract period, this program has resulted in two refereed publications in the literature and three more are in the process. Reprints of these publications supported by ARO have been sent to the program manager under separate cover:

J. He and G. J. Iafrate, "Effects of Band Structure and Electric Fields on Resonant Tunneling Dynamics," in Quantum Transport in Ultrasmall Devices, edited by D. K. Ferry et al. (Plenum, New York, 1995), NATO ASI Series B: Physics, Vol. 342, p. 281.

J. He and G. J. Iafrate, "Quantum Properties of Bloch Electrons in Spatially Homogeneous Electric Field," in Hot Carriers in Semiconductors, edited by K. Hess, J.-P. Leburton, and U. Ravaioli (Plenum, New York, 1996), pp. 147-152.

J. He and G. J. Iafrate, "Transport and Absorption properties of a Periodic Crystal in a Superimposed Uniform and Oscillatory Electric Field," to be published.

J. He and G. J. Iafrate, "Multiband Transitions in Solid due to Spatially Homogeneous, Time-Dependent Electric Field, to be published.

J. He and G. J. Iafrate, "Variational Principles for the Time-Dependent Barrier Transmission in a Spatially Homogeneous Electric Field," to be published.